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Chemical Science (electronic: ISSN 2041-6539) is published 48 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK.

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# Chemical Science

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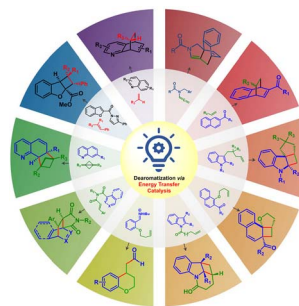


## REVIEWS

12004

## Rejuvenation of dearomative cycloaddition reactions via visible light energy transfer catalysis

Angshuman Palai, Pramod Rai and Biplab Maji\*

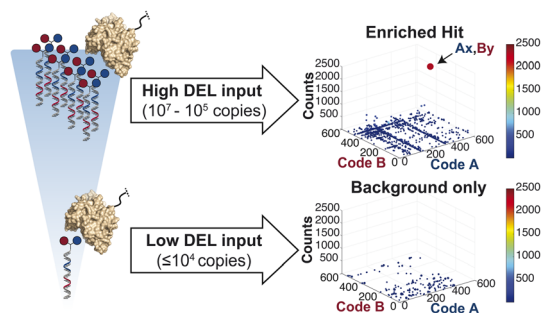


## EDGE ARTICLES

12026

## Impact of library input on the hit discovery rate in DNA-encoded chemical library selections

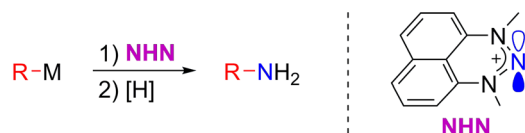
Sara Puglioli, Sebastian Oehler, Luca Prati, Jörg Scheuermann, Gabriele Bassi, Samuele Cazzamalli, Dario Neri\* and Nicholas Favalli\*



12034

## Nitrenium ions as new versatile reagents for electrophilic amination

Idan Avigdori, Kuldeep Singh, Natalia Fridman and Mark Gandelman\*

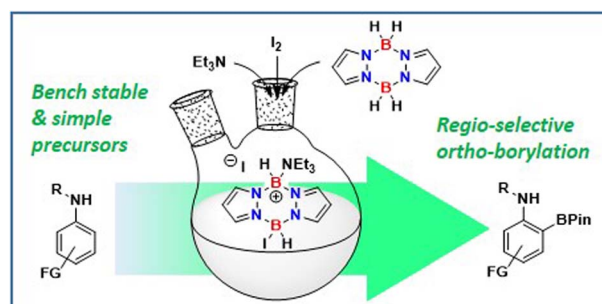


- ✓ *R* = 1°, 2°, 3° **alkyl** and diversely substituted **aryl** groups
- ✓ **Bench-stable**, non-oxidizing, easily prepared aminating agent
- ✓ One-pot synthesis of <sup>15</sup>**N-labelled** biologically relevant amines
- ✓ Simple **recycling** procedure for the aminating agent

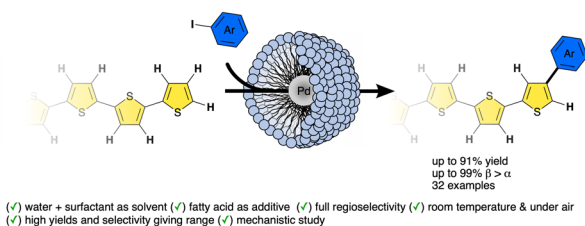
12041

Borylation directed borylation of *N*-alkyl anilines using iodine activated pyrazoboles

C. R. P. Millet, E. Noone, A. V. Schellbach, J. Pahl, J. Łosiewicz, G. S. Nichol and M. J. Ingleson\*



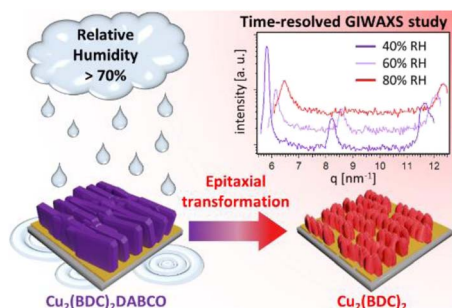
12049



### Micellar catalysis: a green solution to enable undirected and mild C–H activation of (oligo) thiophenes at the challenging $\beta$ -position

Pascal Hauk, Valérie Mazan, Fabrice Gallou\* and Joanna Wencel-Delord\*

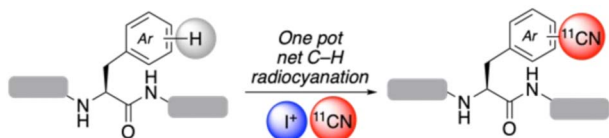
12056



### Water sensitivity of heteroepitaxial Cu-MOF films: dissolution and re-crystallization of 3D-oriented MOF superstructures

Lea A. Brandner, Mercedes Linares-Moreau, Guojun Zhou, Heinz Amenitsch, Simone Dal Zilio, Zhehao Huang, Christian Doonan\* and Paolo Falcaro\*

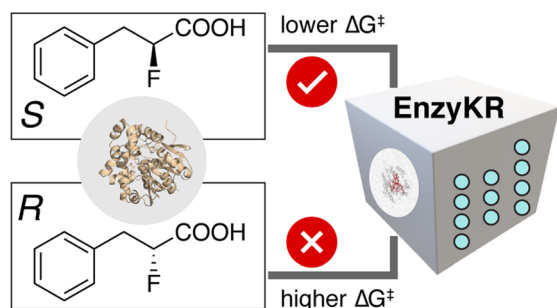
12068



### C–H radiocyanation of bioactive molecules *via* sequential iodination/copper-mediated cross-coupling

Mami Horikawa, Stephen T. Joy, Liam S. Sharninghausen, Xia Shao, Anna K. Mapp,\* Peter J. H. Scott\* and Melanie S. Sanford\*

12073



### EnzyKR: a chirality-aware deep learning model for predicting the outcomes of the hydrolase-catalyzed kinetic resolution

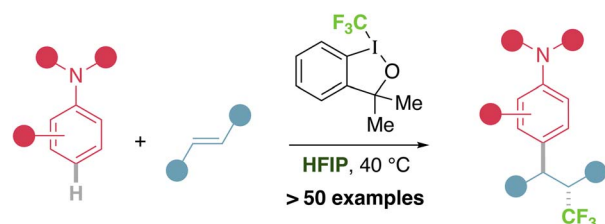
Xinchun Ran, Yaoyukun Jiang, Qianzhen Shao and Zhongyue J. Yang\*



12083

## Trifluoromethylarylation of alkenes using anilines

Carlos Corral Suarez and Ignacio Colomer\*



- ✓ metal- and photocatalyst-free
- ✓ chemo- regio- and stereocontrol
- ✓ mechanistic studies
- ✓ drug functionalization

12091

Organocatalytic atroposelective synthesis of axially chiral *N,N'*-pyrrolylindoles via *de novo* indole formation

Cong-Shuai Wang, Qi Xiong, Hui Xu, Hao-Ran Yang, Yanfeng Dang,\* Xiu-Qin Dong\* and Chun-Jiang Wang\*

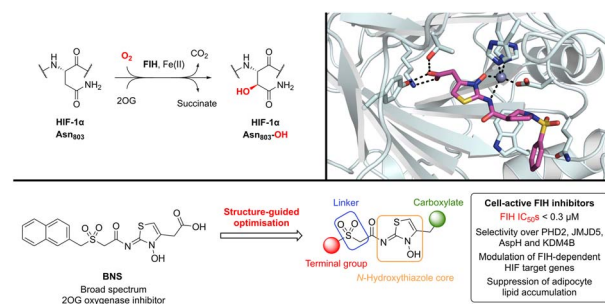


- ★ *N,N'*-pyrrolylindoles atropisomers
- ★ asymmetric 5-*endo-dig* cyclization
- ★ wide substrate scope, exclusive regioselectivity, excellent enantioselectivity

12098

Structure-guided optimisation of *N*-hydroxythiazole-derived inhibitors of factor inhibiting hypoxia-inducible factor- $\alpha$ 

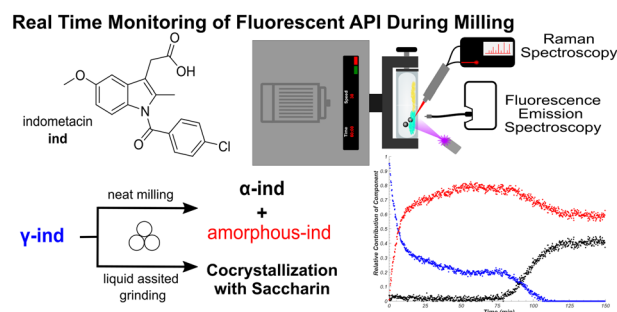
Thomas P. Corner, Ryan Z. R. Teo, Yue Wu, Eidarus Salah, Yu Nakashima, Giorgia Fiorini, Anthony Tumber, Amelia Brasnett, James P. Holt-Martyn, William D. Figg, Jr., Xiaojin Zhang,\* Lennart Brewitz\* and Christopher J. Schofield\*



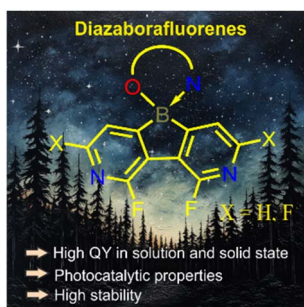
12121

## Illuminating milling mechanochemistry by tandem real-time fluorescence emission and Raman spectroscopy monitoring

Patrick A. Julien,\* Mihails Arhangelskis,\* Luzia S. Germann, Martin Etter, Robert E. Dinnebier, Andrew J. Morris\* and Tomislav Friščić\*



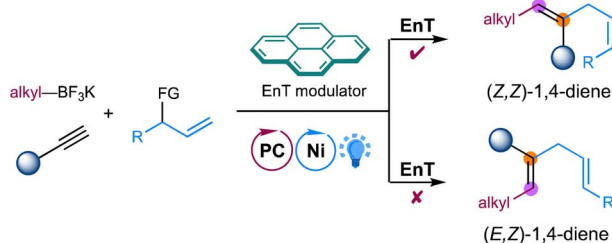
12133



### Highly electron-deficient 3,6-diaza-9-borafluorene scaffolds for the construction of luminescent chelate complexes

Jan Adamek, Paulina H. Marek-Urban, Krzysztof Woźniak, Krzysztof Durka\* and Sergiusz Luliński\*

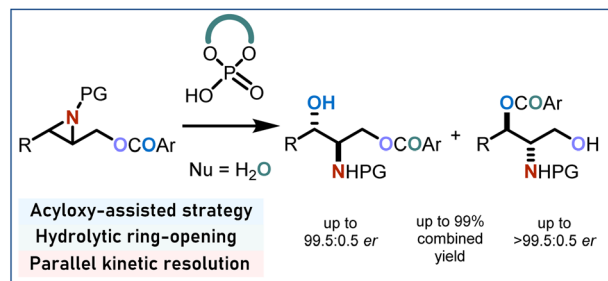
12143



### Divergent 1,2-carboallylation of terminal alkynes enabled by metallaphotoredox catalysis with switchable triplet energy transfer

Jian Qin, Zhuzhu Zhang, Yi Lu, Shengqing Zhu and Lingling Chu\*

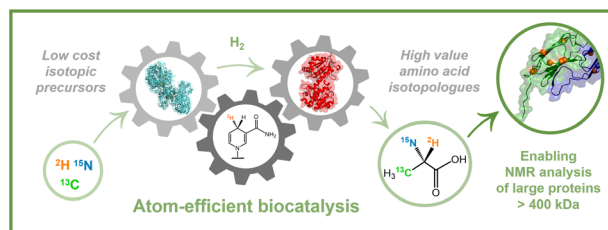
12152



### Parallel kinetic resolution of aziridines via chiral phosphoric acid-catalyzed apparent hydrolytic ring-opening

Juan Liu, Yi-Ying Du, Yu-Shi He, Yan Liang, Shang-Zhong Liu, Yi-Yi Li and Yi-Ming Cao\*

12160



### Biocatalytic reductive amination as a route to isotopically labelled amino acids suitable for analysis of large proteins by NMR

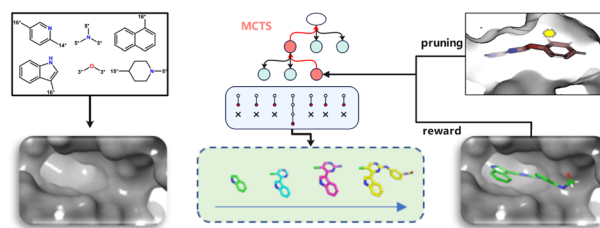
Jack S. Rowbotham,\* Jake H. Nicholson, Miguel A. Ramirez, Kouji Urata, Peter M. T. Todd, Gogulan Karunanithy, Lars Lauterbach, Holly A. Reeve, Andrew J. Baldwin\* and Kylie A. Vincent\*



12166

### A flexible data-free framework for structure-based *de novo* drug design with reinforcement learning

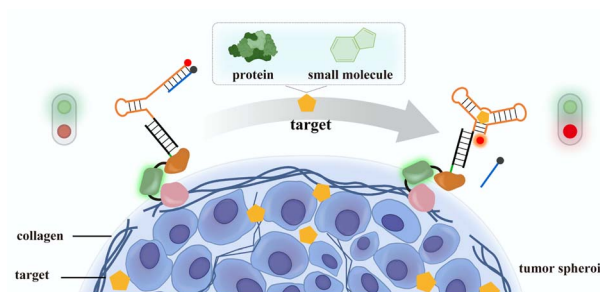
Hongyan Du, Dejun Jiang, Odin Zhang, Zhenxing Wu, Junbo Gao, Xujun Zhang, Xiaorui Wang, Yafeng Deng, Yu Kang, Dan Li, Peichen Pan,\* Chang-Yu Hsieh\* and Tingjun Hou\*



12182

### A collagen-immobilized nanodevice for *in situ* ratiometric imaging of cancer biomarkers in the tumor microenvironment

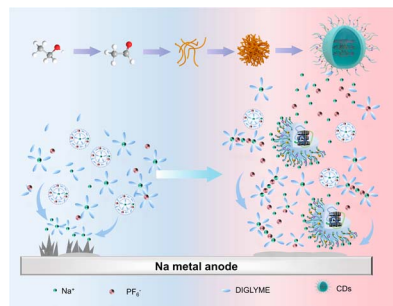
Fengyu Tian, Shurui Zhou, Shiyi Xie, Zhenhua Zhang, Ling Peng, Ling Jiang, Zeyuan Wang, Zhou Nie and Yan Huang\*



12194

### Carbon dots from alcohol molecules: principles and the reaction mechanism

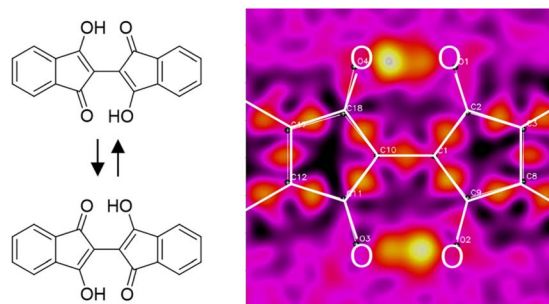
Hanyu Tu, Huaxin Liu, Laiqiang Xu, Zheng Luo, Lin Li, Ye Tian, Wentao Deng, Guoqiang Zou, Hongshuai Hou\* and Xiaobo Ji\*



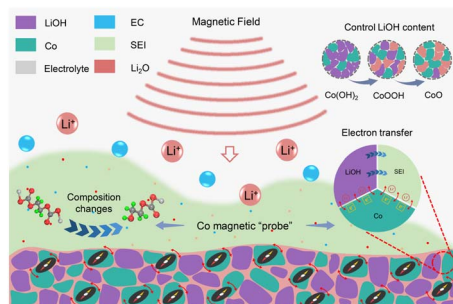
12205

### Synthesis of 3,3'-dihydroxy-2,2'-diindan-1,1'-dione derivatives for tautomeric organic semiconductors exhibiting intramolecular double proton transfer

Kyohei Nakano, Iat Wai Leong, Daisuke Hashizume, Kirill Bulgarevich, Kazuo Takimiya, Yusuke Nishiyama, Toshio Yamazaki and Keisuke Tajima\*



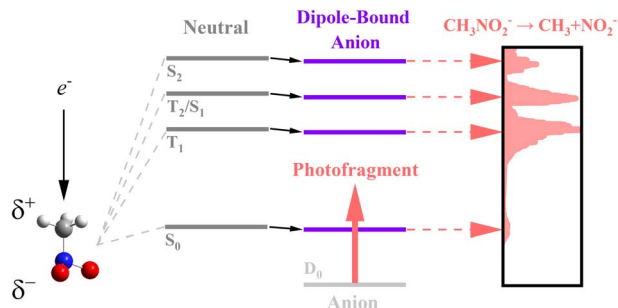
12219



### Revealing the effect of LiOH on forming a SEI using a Co magnetic “probe”

Zhiqiang Zhao, Wanneng Ye, Fengling Zhang, Yuanyuan Pan, Zengqing Zhuo, Feihu Zou, Xixiang Xu, Xiancheng Sang, Weiqi Song, Yue Zhao, Hongsen Li, Kuikui Wang, Chunfu Lin, Han Hu,\* Qinghao Li,\* Wanli Yang and Qiang Li\*

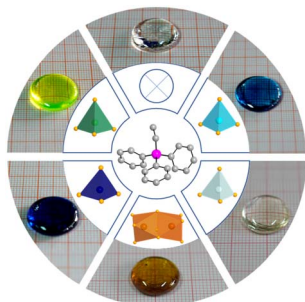
12231



### Excited-state chemistry of the nitromethane anion mediated by the dipole-bound states revealed by photofragment action spectroscopy

Sejun An, Dabin Kim, Junggil Kim and Sang Kyu Kim\*

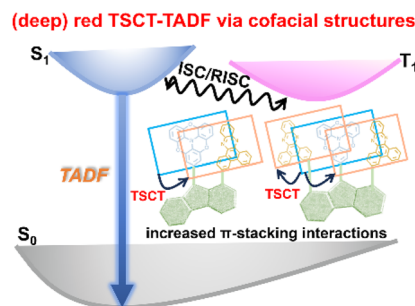
12238



### In situ recrystallization of zero-dimensional hybrid metal halide glass-ceramics toward improved scintillation performance

Bohan Li, Jiance Jin, Meijuan Yin, Kai Han, Yuchi Zhang, Xinlei Zhang, Anran Zhang, Zhiguo Xia\* and Yan Xu\*

12246



### Simultaneously enhancing the planarity and electron-donating capability of donors for through-space charge transfer TADF towards deep-red emission

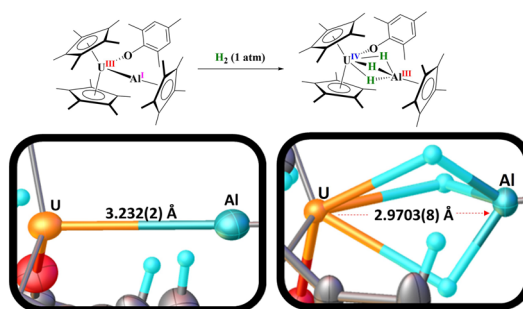
Xiu-Fang Song, Chenglin Jiang, Nengquan Li, Jingsheng Miao, Kai Li\* and Chuluo Yang\*



12255

### Cooperative dihydrogen activation with unsupported uranium–metal bonds and characterization of a terminal U(IV) hydride

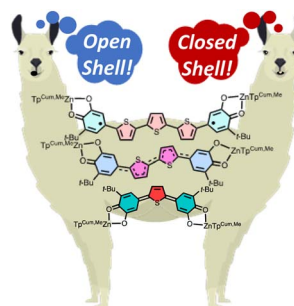
Robert J. Ward, Pokpong Rungthanaphatsophon, Patrick Huang, Steven P. Kelley and Justin R. Walensky\*



12264

### Variation from closed-shell to open shell electronic structures in oligothiophene bis(dioxolene) complexes

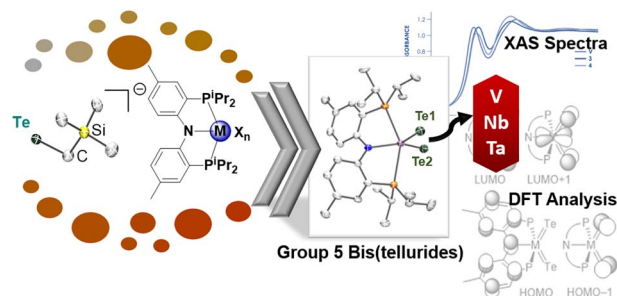
Paul D. Miller, David A. Shultz,\* Joshua Mengell, Martin L. Kirk\* and Lukasz Wojtas



12277

### Tellurolate: an effective Te-atom transfer reagent to prepare the triad of group 5 metal bis(tellurides)

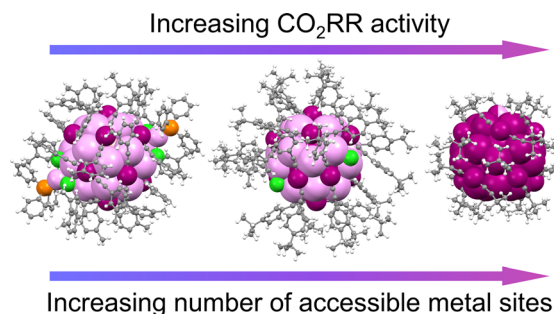
Shuruthi Senthil, Seongyeon Kwon, Richard Y. Kong, Samantha N. MacMillan, Pavel Zatsepin, Michael R. Gau, Patrick J. Carroll, Mu-Hyun Baik,\* Kyle M. Lancaster\* and Daniel J. Mindiola\*



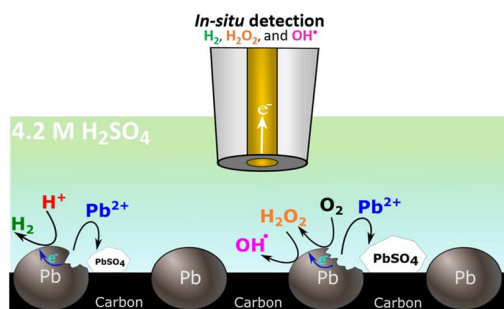
12283

### The role of metal accessibility on carbon dioxide electroreduction in atomically precise nanoclusters

Yingwei Li, Grant J. Stec, Agnes E. Thorarinsdottir, Ryan D. McGillicuddy, Shao-Liang Zheng and Jarad A. Mason\*



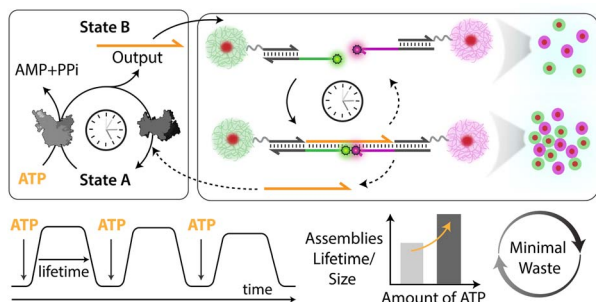
12292



### **In situ** detection of reactive oxygen species spontaneously generated on lead acid battery anodes: a pathway for degradation and self-discharge at open circuit

Abdelilah Asserghine, Aravind Baby, Seth T. Putnam, Peisen Qian, Elizabeth Gao, Huimin Zhao and Joaquín Rodríguez-López\*

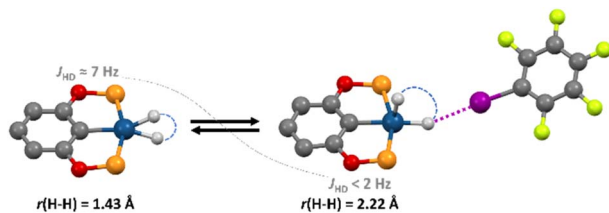
12299



### Transient co-assemblies of micron-scale colloids regulated by ATP-fueled reaction networks

Charu Sharma, Aritra Sarkar and Andreas Walther\*

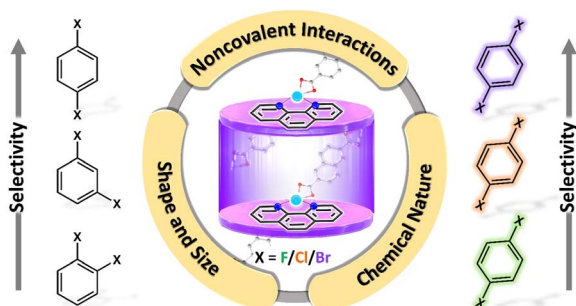
12308



### Unravelling strong temperature-dependence of $J_{\text{HD}}$ in transition metal hydrides: solvation and non-covalent interactions *versus* temperature-elastic H-H bonds

Alexey V. Polukeev,\* Silvia C. Capelli and Ola F. Wendt

12321



### Noncovalent interaction guided selectivity of haloaromatic isomers in a flexible porous coordination polymer

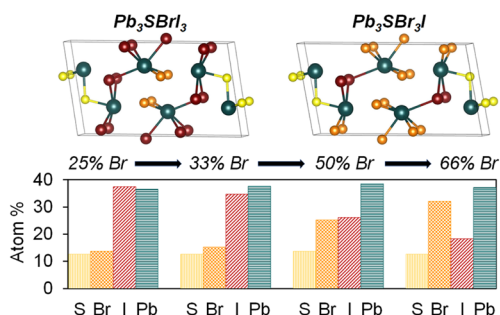
Rohan Jena, Subhajit Laha, Nimish Dwarkanath, Arpan Hazra, Ritesh Halder,\* Sundaram Balasubramanian\* and Tapas Kumar Maji\*



12331

### Designing complex $Pb_3SBr_xI_{4-x}$ chalcogenides: tunable emission semiconductors through halide-mixing

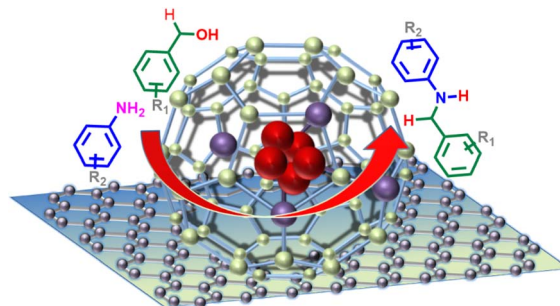
Alison N. Roth, Yunhua Chen, Anuluxan Santhiran, Jemima Opare-Addo, Eunbyeol Gi, Emily A. Smith, Aaron J. Rossini and Javier Vela\*



12339

### Metal-organic framework-derived $CoN_x$ nanoparticles on N-doped carbon for selective *N*-alkylation of aniline

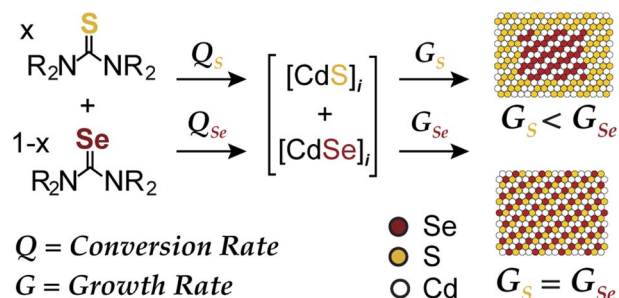
Ved Vyas, Priyanka Maurya and Arindam Indra\*



12345

### Synthesis of graded $CdS_{1-x}Se_x$ nanoplatelet alloys and heterostructures from pairs of chalcogenoureas with tailored conversion reactivity

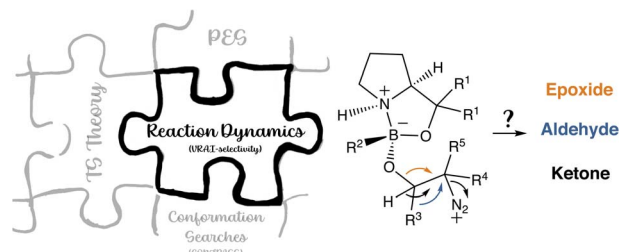
Natalie Saenz, Leslie S. Hamachi, Anna Wolock, Berit H. Goodge, Alexis Kuntzmann, Benoit Dubertret, Isabel Billinge, Lena F. Kourkoutis, David A. Muller, Andrew C. Crowther and Jonathan S. Owen\*



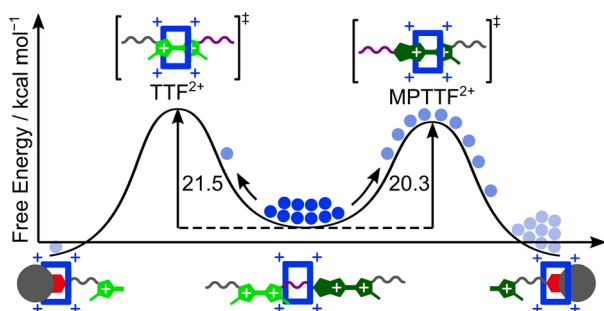
12355

### Reaction dynamics as the missing puzzle piece: the origin of selectivity in oxazaborolidinium ion-catalysed reactions

Ching Ching Lam and Jonathan M. Goodman



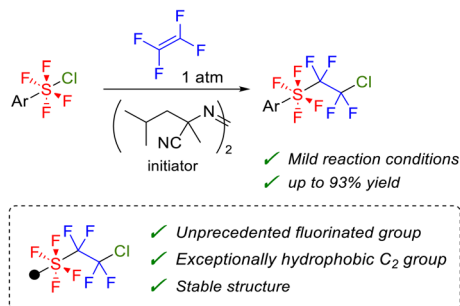
12366



### Mechanistic studies of isomeric [2]rotaxanes consisting of two different tetrathiafulvalene units reveal that the movement of cyclobis(paraquat-*p*-phenylene) can be controlled

Sofie K. Jensen, Mathias S. Neumann, Rikke Frederiksen, Mathias L. Skavenborg, Mads C. Larsen, Stinne E. Wessel and Jan O. Jeppesen\*

12379



### Fluoroalkylated hypervalent sulfur fluorides: radical addition of arylchlorotetrafluoro- $\lambda^6$ -sulfanes to tetrafluoroethylene

Eisuke Yasuo, Kohsuke Aikawa,\* Kyoko Nozaki and Takashi Okazoe

## CORRECTION

12386

### Correction: Structurally divergent enantioselective synthesis of benzofuran fused azocine derivatives and spiro-cyclopentanone benzofurans enabled by sequential catalysis

Rupkumar Khuntia, Sanat Kumar Mahapatra, Lisa Roy and Subhas Chandra Pan\*

